

Generative Models as an Emerging Paradigm in the Chemical Sciences

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Abstract

Traditional computational approaches to design chemical species are limited by the need to compute properties for a vast number of candidates, e.g., by discriminative modeling. Therefore, inverse design methods aim to start from the desired property and optimize a corresponding chemical structure. From a machine learning viewpoint, the inverse design problem can be addressed through so-called generative modeling. Mathematically, discriminative models are defined by learning the probability distribution function of properties given the molecular or material structure. In contrast, a generative model seeks to exploit the joint probability of a chemical species with target characteristics. The overarching idea of generative modeling is to implement a system that produces novel compounds that are expected to have a desired set of chemical features, effectively sidestepping issues found in the forward design process. In this contribution, we overview and critically analyze popular generative algorithms like generative adversarial networks, variational autoencoders, flow, and diffusion models. We highlight key differences between each of the models, provide insights into recent success stories, and discuss outstanding challenges for realizing generative modeling discovered solutions in chemical applications.